

Global Quantum Discord in Multipartite Systems

C. C. Rulli* and M. S. Sarandy†

*Instituto de Física, Universidade Federal Fluminense,
Av. Gal. Milton Tavares de Souza s/n, Gragoatá, 24210-346, Niterói, RJ, Brazil.*

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We propose a global measure for quantum correlations in multipartite systems, which is obtained by suitably recasting the quantum discord in terms of relative entropy and local von Neumann measurements. The measure is symmetric with respect to subsystem exchange and is shown to be non-negative for an arbitrary state. As an illustration, we consider tripartite correlations in the Werner-GHZ state and multipartite correlations at quantum criticality. In particular, in contrast with the pairwise quantum discord, we show that the global quantum discord is able to characterize the infinite-order quantum phase transition in the Ashkin-Teller spin chain.

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I. INTRODUCTION

Quantum correlations constitute a fundamental resource for quantum information tasks [1]. They are rooted in the superposition principle, displaying effects with no classical analog. The research on quantum correlation measures was initially developed based on the entanglement-separability paradigm [2]. More recently, however, it has been perceived that entangled states are not the only kind of quantum states exhibiting non-classical features. In this context, a suitable measure of quantum correlation has been introduced by Ollivier and Zurek [3]. This measure, which has been designated as *quantum discord*, is able to capture not only quantum correlations in entangled states but also in separable states. It arises as a difference between two expressions for the total correlation in a bipartite system (as measured by the mutual information), which are classically equivalent but distinct in the quantum regime. Remarkably, quantum discord has been revealed as a useful quantity in a number of applications, such as quantum critical phenomena [4, 5] and quantum evolution under decoherence [6]. Moreover, quantum discord has also been conjectured to be a resource for speed up in quantum computation [7] and for locking classical correlations in quantum states [8].

In recent years, generalizations of quantum discord to multipartite states have been considered in different scenarios [9]. One possible approach is based on directly generalizing the quantum mutual information to a multipartite system, even though nonunique generalizations are possible in this situation [10, 11]. Another approach is to define from the beginning a measure based on the relative entropy, which allows for a unified view of different correlation sources, such as entanglement, quantum discord, and dissonance [12] (see also Ref. [13]). The aim of this work is to propose a global measure of quantum discord obtained by a systematic extension of the

bipartite quantum discord, with operational appeal and satisfying the basic requirements of a correlation function. In this direction, we suitably recast the standard bipartite quantum discord defined in Ref. [3] in terms of relative entropy and local von Neumann measurements, whence a natural multipartite measure for quantum correlations emerges. This measure – named here as *global quantum discord* (GQD) – is symmetric with respect to subsystem exchange and shown to be non-negative for arbitrary states. We illustrate our results by computing the tripartite GQD in the Werner-GHZ state and by applying GQD in the characterization of the infinite-order quantum phase transition (QPT) in the Ashkin-Teller spin chain, where ordinary pairwise quantum discord fails.

II. QUANTUM DISCORD

Consider a bipartite system AB composed of subsystems A and B . Denoting by $\hat{\rho}_{AB}$ the density operator of AB and by $\hat{\rho}_A$ and $\hat{\rho}_B$ the density operator of parts A and B , respectively, the total correlation between A and B is measured by the quantum mutual information

$$I(\hat{\rho}_{AB}) = S(\hat{\rho}_A) - S(\hat{\rho}_A|\hat{\rho}_B), \quad (1)$$

where $S(\hat{\rho}_A) = -\text{Tr} \hat{\rho}_A \log_2 \hat{\rho}_A$ is the von Neumann entropy for A and

$$S(\hat{\rho}_A|\hat{\rho}_B) = S(\hat{\rho}_{AB}) - S(\hat{\rho}_B) \quad (2)$$

is the entropy of A conditional on B . The conditional entropy can also be introduced by a measurement-based approach. Indeed, consider a measurement locally performed on B , which can be described by a set of projectors $\{\hat{\Pi}_B^j\} = \{|b_j\rangle\langle b_j|\}$. The state of the quantum system, conditioned on the measurement of the outcome labeled by j , is

$$\hat{\rho}_{AB|j} = \frac{1}{p_j} \left(\hat{\mathbf{1}}_A \otimes \hat{\Pi}_B^j \right) \hat{\rho}_{AB} \left(\hat{\mathbf{1}}_A \otimes \hat{\Pi}_B^j \right), \quad (3)$$

where $p_j = \text{Tr}[(\hat{\mathbf{1}}_A \otimes \hat{\Pi}_B^j)\hat{\rho}_{AB}(\hat{\mathbf{1}}_A \otimes \hat{\Pi}_B^j)]$ denotes the probability of obtaining the outcome j and $\hat{\mathbf{1}}_A$ denotes

* clodoalrulli@gmail.com

† msarandy@if.uff.br

the identity operator for A . The conditional density operator $\hat{\rho}_{AB|j}$ allows for the following alternative definition of the conditional entropy:

$$S(\hat{\rho}_{AB}|\{\hat{\Pi}_B^j\}) = \sum_j p_j S(\hat{\rho}_{A|j}), \quad (4)$$

where $\hat{\rho}_{A|j} = \text{Tr}_B \hat{\rho}_{AB|j} = (1/p_j) \langle b_j | \hat{\rho}_{AB} | b_j \rangle$, with $S(\hat{\rho}_{A|j}) = S(\hat{\rho}_{AB|j})$. Therefore, the quantum mutual information can also be defined by

$$J(\hat{\rho}_{AB}) = S(\hat{\rho}_A) - S(\hat{\rho}_{AB}|\{\hat{\Pi}_B^j\}). \quad (5)$$

The quantities $I(\hat{\rho}_{AB})$ and $J(\hat{\rho}_{AB})$ are classically equivalent but they are distinct in the quantum case. This difference is the quantum discord $\overline{\mathcal{D}}(\hat{\rho}_{AB})$ [3], yielding

$$\overline{\mathcal{D}}(\hat{\rho}_{AB}) = I(\hat{\rho}_{AB}) - J(\hat{\rho}_{AB}). \quad (6)$$

Note that $\overline{\mathcal{D}}(\hat{\rho}_{AB})$ is defined as a non-negative asymmetric quantity that depends on $\{\hat{\Pi}_B^j\}$. This dependence can be eliminated by minimizing $\overline{\mathcal{D}}(\hat{\rho}_{AB})$ over all measurement bases $\{\hat{\Pi}_B^j\}$ [14].

III. RELATIVE ENTROPY AND SYMMETRIC QUANTUM DISCORD

The quantum relative entropy is a measure of distinguishability between two arbitrary density operators $\hat{\rho}$ and $\hat{\sigma}$, which is defined as [15]

$$S(\hat{\rho} \parallel \hat{\sigma}) = \text{Tr}(\hat{\rho} \log_2 \hat{\rho} - \hat{\rho} \log_2 \hat{\sigma}). \quad (7)$$

We can express the quantum mutual information $I(\hat{\rho}_{AB})$ as the relative entropy between $\hat{\rho}_{AB}$ and the product state $\hat{\rho}_A \otimes \hat{\rho}_B$, i.e.

$$I(\hat{\rho}_{AB}) = S(\hat{\rho}_{AB} \parallel \hat{\rho}_A \otimes \hat{\rho}_B). \quad (8)$$

In order to express the measurement-induced quantum mutual information $J(\hat{\rho}_{AB})$ in terms of relative entropy, we need to consider a non-selective von Neumann measurement on part B of $\hat{\rho}_{AB}$, which yields

$$\begin{aligned} \Phi_B(\hat{\rho}_{AB}) &= \sum_j \left(\hat{1}_A \otimes \hat{\Pi}_B^j \right) \hat{\rho}_{AB} \left(\hat{1}_A \otimes \hat{\Pi}_B^j \right) \\ &= \sum_j p_j \hat{\rho}_{A|j} \otimes |b_j\rangle \langle b_j|. \end{aligned} \quad (9)$$

Moreover, tracing over the variables of the subsystem A , we obtain

$$\Phi_B(\hat{\rho}_B) = \Phi_B(\text{Tr}_A \hat{\rho}_{AB}) = \sum_j p_j |b_j\rangle \langle b_j|, \quad (10)$$

where we have used that $\text{Tr}_A(\hat{\rho}_{A|j}) = 1$. Then, by expressing the entropies $S(\Phi_B(\hat{\rho}_{AB}))$ and $S(\Phi_B(\hat{\rho}_B))$ as

$$S(\Phi_B(\hat{\rho}_{AB})) = H(\mathbf{p}) + \sum_j p_j S(\hat{\rho}_{A|j}) \quad (11)$$

and

$$S(\Phi_B(\hat{\rho}_B)) = H(\mathbf{p}), \quad (12)$$

with $H(\mathbf{p})$ denoting the Shannon entropy

$$H(\mathbf{p}) = - \sum_j p_j \log_2(p_j), \quad (13)$$

we can rewrite $J(\hat{\rho}_{AB})$ as

$$\begin{aligned} J(\hat{\rho}_{AB}) &= S(\hat{\rho}_A) - \sum_j p_j S(\hat{\rho}_{A|j}) \\ &= S(\hat{\rho}_A) + S(\Phi_B(\hat{\rho}_B)) - S(\Phi_B(\hat{\rho}_{AB})) \\ &= S(\Phi_B(\hat{\rho}_{AB}) \parallel \hat{\rho}_A \otimes \Phi_B(\hat{\rho}_B)). \end{aligned} \quad (14)$$

Therefore, the quantum discord can be rewritten in terms of a difference of relative entropies:

$$\begin{aligned} \overline{\mathcal{D}}(\hat{\rho}_{AB}) &= S(\hat{\rho}_{AB} \parallel \hat{\rho}_A \otimes \hat{\rho}_B) \\ &\quad - S(\Phi_B(\hat{\rho}_{AB}) \parallel \hat{\rho}_A \otimes \Phi_B(\hat{\rho}_B)), \end{aligned} \quad (15)$$

with minimization taken over $\{\hat{\Pi}_B^j\}$ to remove the measurement-basis dependence. It is possible then to obtain a natural symmetric extension $\mathcal{D}(\hat{\rho}_{AB})$ for the quantum discord $\overline{\mathcal{D}}(\hat{\rho}_{AB})$. Indeed, performing measurements over both subsystems A and B , we define

$$\begin{aligned} \mathcal{D}(\hat{\rho}_{AB}) &= \min_{\{\hat{\Pi}_A^j \otimes \hat{\Pi}_B^k\}} [S(\hat{\rho}_{AB} \parallel \hat{\rho}_A \otimes \hat{\rho}_B) \\ &\quad - S(\Phi_{AB}(\hat{\rho}_{AB}) \parallel \Phi_A(\hat{\rho}_A) \otimes \Phi_B(\hat{\rho}_B))], \end{aligned} \quad (16)$$

where the operator Φ_{AB} is given by

$$\Phi_{AB}(\hat{\rho}_{AB}) = \sum_{j,k} \left(\hat{\Pi}_A^j \otimes \hat{\Pi}_B^k \right) \hat{\rho}_{AB} \left(\hat{\Pi}_A^j \otimes \hat{\Pi}_B^k \right). \quad (17)$$

Observe that, by writing Eq. (16) in terms of the mutual information I , we obtain

$$\mathcal{D}(\hat{\rho}_{AB}) = \min_{\{\hat{\Pi}_A^j \otimes \hat{\Pi}_B^k\}} [I(\hat{\rho}_{AB}) - I(\Phi_{AB}(\hat{\rho}_{AB}))], \quad (18)$$

which is the symmetric version of the expression for the loss of correlation due to measurement [11, 16]. Remarkably, $\mathcal{D}(\hat{\rho}_{AB})$ is equivalent to the measurement-induced disturbance (MID) [17] if measurement is performed in the eigenprojectors of the reduced density operators of each part (instead of minimization). Moreover, Eq. (16) also provides the symmetric quantum discord considered in Ref. [18] and experimentally witnessed in Ref. [19]. As a further step, we can still rearrange Eq. (16) in a rather convenient way, yielding

$$\begin{aligned} \mathcal{D}(\hat{\rho}_{AB}) &= \min_{\{\hat{\Pi}_A^j \otimes \hat{\Pi}_B^k\}} [S(\hat{\rho}_{AB} \parallel \Phi_{AB}(\hat{\rho}_{AB})) \\ &\quad - S(\hat{\rho}_A \parallel \Phi_A(\hat{\rho}_A)) - S(\hat{\rho}_B \parallel \Phi_B(\hat{\rho}_B))]. \end{aligned} \quad (19)$$

IV. GLOBAL QUANTUM DISCORD

Let us now extend quantum discord as given by Eq. (19) to multipartite systems.

Definition. The global quantum discord $\mathcal{D}(\hat{\rho}_{A_1 \dots A_N})$ for an arbitrary multipartite state $\hat{\rho}_{A_1 \dots A_N}$ under a set of local measurements $\{\hat{\Pi}_{A_1}^{j_1} \otimes \dots \otimes \hat{\Pi}_{A_N}^{j_N}\}$ is defined as

$$\mathcal{D}(\hat{\rho}_{A_1 \dots A_N}) = \min_{\{\hat{\Pi}_k\}} [S(\hat{\rho}_{A_1 \dots A_N} \parallel \Phi(\hat{\rho}_{A_1 \dots A_N})) - \sum_{j=1}^N S(\hat{\rho}_{A_j} \parallel \Phi_j(\hat{\rho}_{A_j}))], \quad (20)$$

where $\Phi_j(\hat{\rho}_{A_j}) = \sum_{j'} \hat{\Pi}_{A_j}^{j'} \hat{\rho}_{A_j} \hat{\Pi}_{A_j}^{j'}$ and $\Phi(\hat{\rho}_{A_1 \dots A_N}) = \sum_k \hat{\Pi}_k \hat{\rho}_{A_1 \dots A_N} \hat{\Pi}_k$, with $\hat{\Pi}_k = \hat{\Pi}_{A_1}^{j_1} \otimes \dots \otimes \hat{\Pi}_{A_N}^{j_N}$ and k denoting the index string $(j_1 \dots j_N)$.

Therefore, a classical state can be defined by $\hat{\rho}_{A_1 \dots A_N} = \Phi(\hat{\rho}_{A_1 \dots A_N})$, which is in agreement with the requirement that classical states are not disturbed by suitable local measurements. Indeed, this definition of a classical state implies that $\hat{\rho}_{A_j} = \Phi_j(\hat{\rho}_{A_j})$ for any j , which means $\mathcal{D}(\hat{\rho}_{A_1 \dots A_N}) = 0$. Moreover, observe that, via minimization over the set of projectors $\{\hat{\Pi}_{A_1}^{j_1} \otimes \dots \otimes \hat{\Pi}_{A_N}^{j_N}\}$, we define GQD as a measurement-basis independent quantity. However, as will be illustrated in the Ashkin-Teller chain, other (non-minimizing) bases are also able to provide relevant information about the behavior of quantum correlations in the system (similarly to the original definition of quantum discord in Ref. [3]). In any case, we can show that GQD is non-negative for an arbitrary state.

Theorem. The global quantum discord $\mathcal{D}(\hat{\rho}_{A_1 \dots A_N})$ is non-negative, i.e., $\mathcal{D}(\hat{\rho}_{A_1 \dots A_N}) \geq 0$.

Proof. In order to prove that $\mathcal{D}(\hat{\rho}_{A_1 \dots A_N}) \geq 0$, we associate with each subsystem A_j an ancilla system B_j . Therefore, we will define a composite density operator $\hat{\rho}'_{A_1 \dots A_N; B_1 \dots B_N}$ such that

$$\hat{\rho}'_{A_1 \dots A_N; B_1 \dots B_N} = \sum_k \sum_{k'} \hat{\Pi}_k \hat{\rho}_{A_1 \dots A_N} \hat{\Pi}_{k'} \otimes \hat{\Lambda}_{kk'}, \quad (21)$$

where $\hat{\Lambda}_{kk'} = |B_{j_1}\rangle\langle B_{j'_1}| \otimes \dots \otimes |B_{j_N}\rangle\langle B_{j'_N}|$, with k and k' denoting the index strings $(j_1 \dots j_N)$ and $(j'_1 \dots j'_N)$, respectively. From the monotonicity of the relative entropy under partial trace [20], for any positive operators $\hat{\sigma}_{12}$ and $\hat{\gamma}_{12}$ such that $\text{Tr}(\hat{\sigma}_{12}) = \text{Tr}(\hat{\gamma}_{12})$, we have that $S(\hat{\sigma}_{12} \parallel \hat{\gamma}_{12}) \geq S(\hat{\sigma}_1 \parallel \hat{\gamma}_1)$, where $\hat{\sigma}_1 = \text{Tr}_2(\hat{\sigma}_{12})$ and $\hat{\gamma}_1 = \text{Tr}_2(\hat{\gamma}_{12})$. Then $S(\hat{\sigma}_{123 \dots N} \parallel \hat{\gamma}_{123 \dots N}) \geq \dots \geq S(\hat{\sigma}_{123} \parallel \hat{\gamma}_{123}) \geq S(\hat{\sigma}_{12} \parallel \hat{\gamma}_{12}) \geq S(\hat{\sigma}_1 \parallel \hat{\gamma}_1)$. By taking $\hat{\rho}'_{A_1 \dots A_N; B_1 \dots B_N}$ as $\hat{\sigma}$ and $\hat{\rho}_{A_1; B_1} \otimes \hat{\rho}'_{A_2; B_2} \otimes \dots \otimes \hat{\rho}'_{A_N; B_N}$ as $\hat{\gamma}$, we obtain

$$S(\hat{\rho}'_{A_1 \dots A_N; B_1 \dots B_N} \parallel \hat{\rho}'_{A_1; B_1} \otimes \hat{\rho}'_{A_2; B_2} \otimes \dots \otimes \hat{\rho}'_{A_N; B_N}) \geq S(\hat{\rho}'_{A_1 \dots A_N} \parallel \hat{\rho}'_{A_1} \otimes \dots \otimes \hat{\rho}'_{A_N}), \quad (22)$$

which, from Eq. (8), implies that

$$\begin{aligned} & \sum_{j=1}^N S(\hat{\rho}'_{A_j; B_j}) - S(\hat{\rho}'_{A_1 \dots A_N; B_1 \dots B_N}) \\ & \geq \sum_{j=1}^N S(\hat{\rho}'_{A_j}) - S(\hat{\rho}'_{A_1 \dots A_N}). \end{aligned} \quad (23)$$

However, from Eq. (21), it follows the relations

$$S(\hat{\rho}'_{A_1 \dots A_N; B_1 \dots B_N}) = S(\hat{\rho}_{A_1 \dots A_N}), \quad (24)$$

$$S(\hat{\rho}'_{A_1 \dots A_N}) = S(\Phi(\hat{\rho}_{A_1 \dots A_N})), \quad (25)$$

$$S(\hat{\rho}'_{A_j; B_j}) = S(\hat{\rho}_{A_j}) \quad (\forall j), \quad (26)$$

$$S(\hat{\rho}'_{A_j}) = S(\Phi_j(\hat{\rho}_{A_j})) \quad (\forall j). \quad (27)$$

Insertion of Eqs.(24)-(27) into inequality (23) yields

$$\begin{aligned} & \sum_{j=1}^N S(\hat{\rho}_{A_j}) - S(\hat{\rho}_{A_1 \dots A_N}) \\ & \geq \sum_{j=1}^N S(\Phi_j(\hat{\rho}_{A_j})) - S(\Phi(\hat{\rho}_{A_1 \dots A_N})). \end{aligned} \quad (28)$$

By rewriting inequality (28) in terms of the relative entropy, we obtain

$$S(\hat{\rho}_{A_1 \dots A_N} \parallel \Phi(\hat{\rho}_{A_1 \dots A_N})) - \sum_{j=1}^N S(\hat{\rho}_{A_j} \parallel \Phi_j(\hat{\rho}_{A_j})) \geq 0. \quad (29)$$

The left hand side of the inequality above is exactly the GQD, as defined by Eq.(20). Hence, $\mathcal{D}(\hat{\rho}_{A_1 \dots A_N}) \geq 0$. ■

V. TRIPARTITE CORRELATIONS IN THE WERNER-GHZ STATE

As a first illustration of GQD, we will consider the Werner-GHZ state

$$\hat{\rho} = \frac{(1-\mu)}{8} \hat{\mathbf{1}} + \mu |GHZ\rangle\langle GHZ|, \quad (30)$$

where $0 \leq \mu \leq 1$ and

$$|GHZ\rangle = (|\uparrow\rangle_A |\uparrow\rangle_B |\uparrow\rangle_C + |\downarrow\rangle_A |\downarrow\rangle_B |\downarrow\rangle_C) / \sqrt{2}, \quad (31)$$

with $|\uparrow\rangle$ and $|\downarrow\rangle$ denoting the eigenstates of the Pauli operator $\hat{\sigma}^z$ associated with eigenvalues 1 and -1, respectively. The Werner-GHZ state provides an interpolation between a fully mixed (uncorrelated) state and a maximally correlated pure tripartite state. It is a rather suitable state to begin with as we propose a measure for quantum correlation and constitutes an interesting scenario to compare multipartite with bipartite correlations, since it is a generalization of the two-qubit Werner state [21]. Let us begin by analyzing GQD in the case of a pure GHZ state ($\mu = 1$).

A. GQD for the GHZ state

Let us focus here on the *GHZ* state, as defined by Eq. (31). In order to define local measurements for $|GHZ\rangle$, let us consider rotations in the directions of the basis vectors of subsystems A , B , and C , which are denoted by

$$|+\rangle_j = \cos\left(\frac{\theta_j}{2}\right) |\uparrow\rangle_j + e^{i\varphi_j} \sin\left(\frac{\theta_j}{2}\right) |\downarrow\rangle_j, \quad (32)$$

$$|-\rangle_j = -e^{-i\varphi_j} \sin\left(\frac{\theta_j}{2}\right) |\uparrow\rangle_j + \cos\left(\frac{\theta_j}{2}\right) |\downarrow\rangle_j, \quad (33)$$

with $j = 1, 2, 3$ for subsystems A , B , and C , respectively. The angles θ_i take values in the interval $[0, \pi)$ and the angles φ_i take values in the interval $[0, 2\pi)$. In order to compute $\mathcal{D}(\hat{\rho})$, with $\hat{\rho} = |GHZ\rangle\langle GHZ|$, we must evaluate the expression

$$\mathcal{D}(\hat{\rho}) = \min_{\theta_i, \varphi_i} [S(\hat{\rho} \parallel \Phi(\hat{\rho})) - S(\hat{\rho}_A \parallel \Phi_A(\hat{\rho}_A)) - S(\hat{\rho}_B \parallel \Phi_B(\hat{\rho}_B)) - S(\hat{\rho}_C \parallel \Phi_C(\hat{\rho}_C))]. \quad (34)$$

However, $S(\hat{\rho}) = 0$, since $\hat{\rho}$ is pure. Moreover, $S(\hat{\rho}_A \parallel \Phi_A(\hat{\rho}_A)) = S(\hat{\rho}_B \parallel \Phi_B(\hat{\rho}_B)) = S(\hat{\rho}_C \parallel \Phi_C(\hat{\rho}_C)) = 0$, since $\hat{\rho}_A$, $\hat{\rho}_B$, and $\hat{\rho}_C$ are proportional to identity operators. Hence, GQD is simply given by

$$\mathcal{D}(\hat{\rho}) = \min_{\theta_i, \varphi_i} S(\Phi(\hat{\rho})) = \min_{\theta_i, \varphi_i} \left[-\sum_j \lambda_j \log_2 \lambda_j \right], \quad (35)$$

where λ_j are the eigenvalues of the operator $\Phi(\hat{\rho})$. They can be obtained from projections of the GHZ state over the rotated basis states. In order to minimize $S(\Phi(\hat{\rho}))$, we must find out the measurement basis that maximizes the purity of $\Phi(\hat{\rho})$, i.e., that maximizes the dispersion of the eigenvalues λ_j with respect to the average of $\{\lambda_j\}$. This is obtained for $\theta_i = 0$ ($i=1,2,3$), namely, measurements in the eigenprojectors of σ_i^z . As an illustration, let us consider the case of $\theta_1 = 0$ and $\varphi_i = 0$ ($i=1,2,3$). In this situation, the eigenvalues λ_j for the operator $\Phi(\hat{\rho})$ read

$$\lambda_1 = \lambda_8 = \frac{1}{2} \cos^2\left(\frac{\theta_2}{2}\right) \cos^2\left(\frac{\theta_3}{2}\right), \quad (36)$$

$$\lambda_2 = \lambda_7 = \frac{1}{2} \cos^2\left(\frac{\theta_2}{2}\right) \sin^2\left(\frac{\theta_3}{2}\right), \quad (37)$$

$$\lambda_3 = \lambda_6 = \frac{1}{2} \sin^2\left(\frac{\theta_2}{2}\right) \cos^2\left(\frac{\theta_3}{2}\right), \quad (38)$$

$$\lambda_4 = \lambda_5 = \frac{1}{2} \sin^2\left(\frac{\theta_2}{2}\right) \sin^2\left(\frac{\theta_3}{2}\right). \quad (39)$$

By using Eqs. (36)-(39) into Eq. (35), we can directly obtain $\mathcal{D}(\hat{\rho})$ by minimizing over the angles θ_2 and θ_3 . The function $D(\theta_2, \theta_3)$ to be minimized is then

$$D(\theta_2, \theta_3) = -\sum_j \lambda_j \log_2 \lambda_j. \quad (40)$$

We plot $D(\theta_2, \theta_3)$ as a function of θ_2 and θ_3 in Fig. 1. Notice that its minimum, which provides $\mathcal{D}(\hat{\rho})$, occurs at the boundary values $\theta_2 = \theta_3 = 0$, where $\mathcal{D}(\hat{\rho}) = 1$. This is a manifestation of the fact that any local measurement disturbs the GHZ state, which is detected by a nonvanishing GQD.

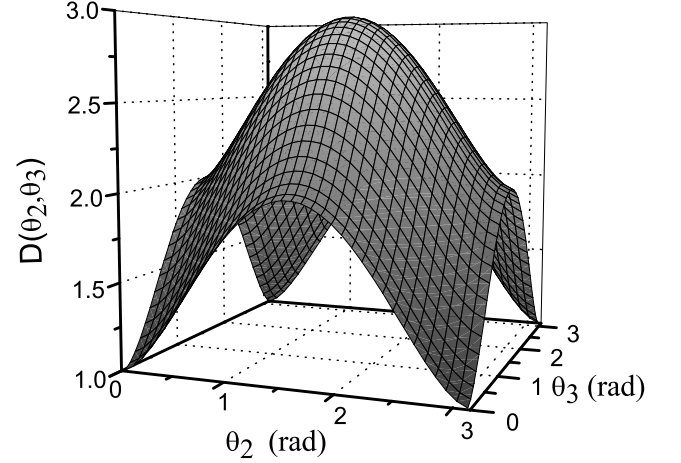


FIG. 1. The function $D(\theta_2, \theta_3)$ as a function of θ_2 and θ_3 . Note that the minimum occurs for $\theta_2 = \theta_3 = 0$, which implies $\mathcal{D}(\hat{\rho}) = 1$.

B. GQD in the Werner-GHZ state

In order to obtain $\mathcal{D}(\hat{\rho})$ for the Werner-GHZ state, let us first rewrite Eq. (30) as

$$\hat{\rho} = \frac{1}{8} \hat{1} + \frac{\mu}{8} (\hat{\sigma}_1^z \hat{\sigma}_2^z + \hat{\sigma}_1^z \hat{\sigma}_3^z + \hat{\sigma}_2^z \hat{\sigma}_3^z + \hat{\sigma}_1^x \hat{\sigma}_2^x \hat{\sigma}_3^x - \hat{\sigma}_1^x \hat{\sigma}_2^y \hat{\sigma}_3^y - \hat{\sigma}_1^y \hat{\sigma}_2^x \hat{\sigma}_3^x - \hat{\sigma}_1^y \hat{\sigma}_2^y \hat{\sigma}_3^z), \quad (41)$$

with σ_i^x , σ_i^y , and σ_i^z denoting the Pauli matrices for the qubit i . Again, we will have here that $S(\hat{\rho}_i \parallel \Phi_i(\hat{\rho}_i)) = 0$ ($i = A, B, C$), since $\hat{\rho}_A$, $\hat{\rho}_B$, and $\hat{\rho}_C$ are proportional to identity operators. Therefore,

$$\mathcal{D}(\hat{\rho}) = \min_{\theta_i, \varphi_i} S(\hat{\rho} \parallel \Phi(\hat{\rho})) = \min_{\theta_i, \varphi_i} [S(\Phi(\hat{\rho})) - S(\hat{\rho})]. \quad (42)$$

The von Neumann entropy $S(\hat{\rho})$ is given by

$$S(\hat{\rho}) = 3 - \frac{7}{8} (1 - \mu) \log_2 (1 - \mu) - \frac{1}{8} (1 + 7\mu) \log_2 (1 + 7\mu). \quad (43)$$

As for the GHZ state, we take local measurements in the $\hat{\sigma}^z$ eigenbasis for each particle to minimize $S(\Phi(\hat{\rho}))$. Such an eigenbasis provides the maximum loss of correlation among the parts of ρ , which therefore minimizes

GQD. Then, from Eq. (41), we obtain

$$\Phi(\hat{\rho}) = \left(\frac{1-\mu}{8}\right) \hat{1} + \frac{\mu}{8} (\hat{1} + \hat{\sigma}_1^z \hat{\sigma}_2^z + \hat{\sigma}_1^z \hat{\sigma}_3^z + \hat{\sigma}_2^z \hat{\sigma}_3^z), \quad (44)$$

which implies

$$S(\Phi(\hat{\rho})) = 3 - \frac{3}{4}(1-\mu) \log_2(1-\mu) - \frac{1}{4}(1+3\mu) \log_2(1+3\mu). \quad (45)$$

Insertion of Eqs. (43) and (45) into Eq. (42) yields

$$\mathcal{D}(\hat{\rho}) = -\frac{1}{4}(1+3\mu) \log_2(1+3\mu) + \frac{1}{8}(1-\mu) \log_2(1-\mu) + \frac{1}{8}(1+7\mu) \log_2(1+7\mu). \quad (46)$$

In Fig. 2 we plot $\mathcal{D}(\hat{\rho})$ as a function of μ . Observe that GQD vanishes only for $\mu = 0$, where $\hat{\rho}$ is a completely mixed state. Moreover, GQD is a monotonic function of μ , acquiring its maximal value $\mathcal{D}(\hat{\rho}) = 1$ for $\mu = 1$, where $\hat{\rho}$ is the GHZ state. This result resembles the behavior of the bipartite Werner state [3, 22].

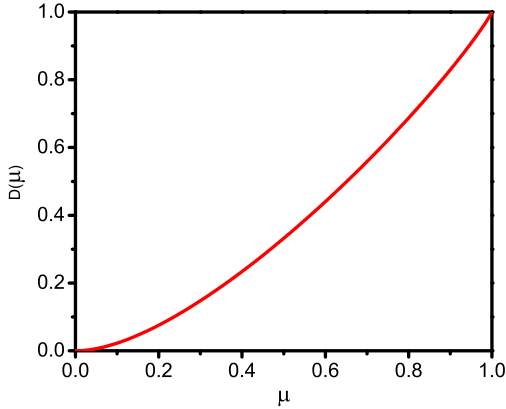


FIG. 2. (Color online) Tripartite GQD for the Werner-GHZ state as a function of the mixing parameter μ . Note that GQD is nonvanishing for $\mu \neq 0$.

VI. MULTIPARTITE CORRELATIONS IN THE ASHKIN-TELLER CHAIN

Let us now present an application of GQD that makes evident the importance of considering genuine multipartite correlations to the characterization of a QPT. In this direction, we consider the Ashkin-Teller model, which has been introduced as a generalization of the Ising spin-1/2 model to investigate the statistics of lattices with four-state interacting sites [23]. It exhibits a rich phase diagram [24] and has recently attracted a great deal of attention due to several interesting applications [25].

The Hamiltonian for the quantum Ashkin-Teller model in one-dimension for a chain with M sites is given by

$$H_{AT} = -J \sum_{j=1}^M (\hat{\sigma}_j^x + \hat{\tau}_j^x + \Delta \hat{\sigma}_j^x \hat{\tau}_j^x) - J\beta \sum_{j=1}^M (\hat{\sigma}_j^z \hat{\sigma}_{j+1}^z + \hat{\tau}_j^z \hat{\tau}_{j+1}^z + \Delta \hat{\sigma}_j^z \hat{\sigma}_{j+1}^z \hat{\tau}_j^z \hat{\tau}_{j+1}^z), \quad (47)$$

where $\hat{\sigma}_j^\alpha$ and $\hat{\tau}_j^\alpha$ ($\alpha = x, y, z$) are independent Pauli spin-1/2 operators, J is the exchange coupling constant, Δ and β are (dimensionless) parameters, and periodic boundary conditions (PBC) are adopted, i.e., $\hat{\sigma}_{M+1}^\alpha = \hat{\sigma}_1^\alpha$ and $\hat{\tau}_{M+1}^\alpha = \hat{\tau}_1^\alpha$ ($\alpha = x, y, z$). The Ashkin-Teller model is $Z_2 \otimes Z_2$ symmetric, with the Hamiltonian commuting with the parity operators

$$\mathcal{P}_1 = \otimes_{j=1}^M \sigma_j^x \quad \text{and} \quad \mathcal{P}_2 = \otimes_{j=1}^M \tau_j^x. \quad (48)$$

Therefore, the eigenspace of H_{AT} can be decomposed into four disjoint sectors labeled by the eigenvalues of \mathcal{P}_1 and \mathcal{P}_2 , namely, $Q = 0$ ($\mathcal{P}_1 = +1, \mathcal{P}_2 = +1$), $Q = 1$ ($\mathcal{P}_1 = +1, \mathcal{P}_2 = -1$), $Q = 2$ ($\mathcal{P}_1 = -1, \mathcal{P}_2 = -1$), and $Q = 3$ ($\mathcal{P}_1 = -1, \mathcal{P}_2 = +1$). By the symmetry of H_{AT} under the interchange $\sigma^\alpha \leftrightarrow \tau^\alpha$, the sectors $Q = 1$ and $Q = 3$ are degenerate. Moreover, we observe that the ground state belongs to the sector $Q = 0$. A schematic view of the Ashkin-Teller chain is shown in Fig. 3. Note that each site contains *two* spin particles, which means that the number N of particles in a chain with M sites is $N = 2M$.

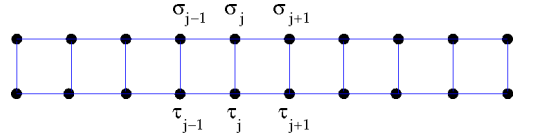


FIG. 3. (Color online) Schematic view of the Ashkin-Teller chain. The lattice is composed by two independent spin-1/2 particles *per* site j described by Pauli operators $\{\sigma_j^\alpha, \tau_j^\alpha\}$.

The model presents an infinite-order quantum critical point at $\beta = 1$ and $\Delta = 1$. Infinite-order QPTs are typically detected by an extremum (either a maximum or a minimum) in quantum correlations measures (see, e.g., Refs. [26, 27] for pairwise entanglement and Ref. [4] for pairwise quantum discord). However, as shown in Ref. [28], pairwise entanglement is unable to characterize the critical point $(\beta, \Delta) = (1, 1)$ in the Ashkin-Teller chain. Moreover, it can be shown that pairwise quantum discord does not detect such a QPT either. Indeed, taking $\beta = 1$, the density operator $\hat{\rho}^{j,j}(\Delta)$ for a pair $\hat{\sigma}_j - \hat{\tau}_j$ is diagonal [28] and exhibits vanishing quantum discord for any Δ . For pairs $\hat{\sigma}_j - \hat{\sigma}_{j+1}$ (or $\hat{\tau}_j - \hat{\tau}_{j+1}$), the density operator $\hat{\rho}^{j,j+1}(\Delta)$ has off-diagonal terms. Such a state displays nonvanishing quantum discord. However, no identification (such as an extremum or a cusp) occurs at the critical point $\Delta = 1$ (for any local measurement).

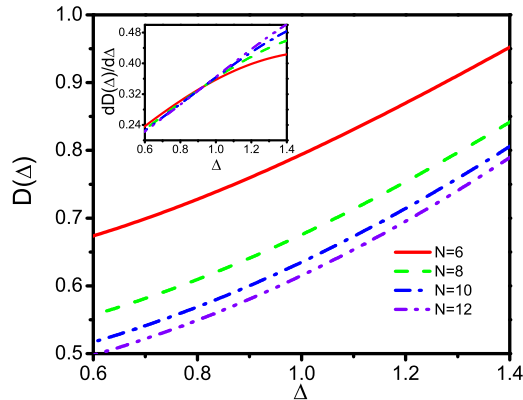


FIG. 4. (Color online) GQD associated with the $\hat{\sigma}^z$ eigenbasis for a spin quartet in the Ashkin-Teller model for chains up to $N = 12$ spins. Inset: Derivative of GQD with respect to Δ .

On the other hand, if we consider multipartite correlations, GQD is able to identify the QPT as an extremum at the critical point. However, such identification does not occur in the basis that minimizes GQD, which is given by the measurement of all spins in the $\hat{\sigma}^z$ eigenbasis. Instead, the infinite-order QPT turns out to be correctly characterized if, and only if, local measurements are performed in the $\hat{\sigma}^x$ eigenbasis. Remarkably, this is exactly the basis of eigenstates of the single spin reduced density operators. Therefore, computation of GQD in such an eigenbasis can be seen as a generalization of MID to the multipartite scenario.

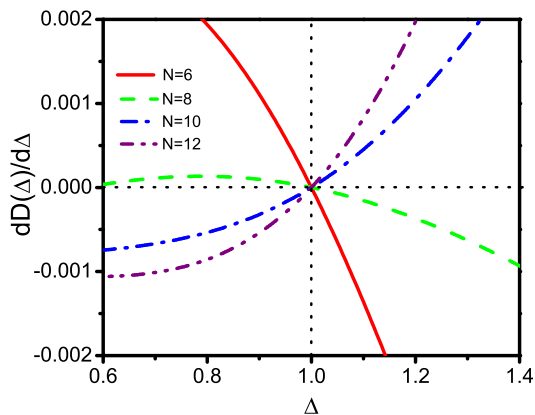


FIG. 5. (Color online) Derivative of GQD associated with the $\hat{\sigma}^x$ eigenbasis for a spin quartet in the Ashkin-Teller model for chains up to $N = 12$ spins.

We consider groups of 4 particles (quartets) composed by spins $\hat{\sigma}_j - \hat{\sigma}_{j+1} - \hat{\tau}_j - \hat{\tau}_{j+1}$ as well as extensions for sextets and octets. For those configurations, we numerically compute GQD relative to local measurements in

the $\hat{\sigma}^z$ eigenbasis and in the $\hat{\sigma}^x$ eigenbasis for each particle via exact diagonalization of chains up to 16 spin

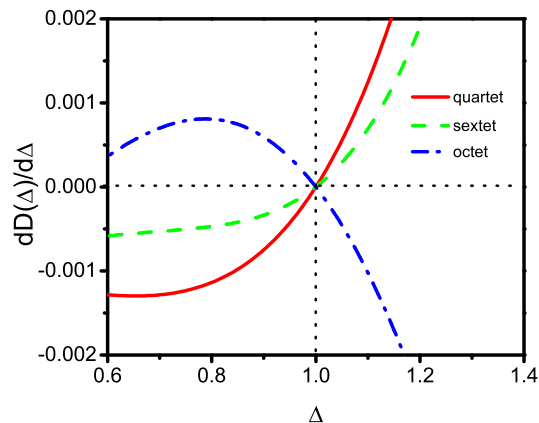


FIG. 6. (Color online) Derivative of GQD associated with the $\hat{\sigma}^x$ eigenbasis for spin quartets, sextets, and octets in the Ashkin-Teller model for a chain with $N = 16$ spins.

particles. The results are exhibited in Fig. 4 for measurements in the $\hat{\sigma}^z$ eigenbasis and in Figs. 5 and 6 for measurements in the $\hat{\sigma}^x$ eigenbasis. We can observe that, in the $\hat{\sigma}^x$ eigenbasis, the identification of the QPT as an extremum (vanishing derivative of the GQD) already occurs for quartets in lattices with $N = 6$ spins (see Fig. 5). Moreover, this characterization is kept for sextets and octets in larger chains (see Fig. 6).

VII. CONCLUSION

In summary, we have proposed a measure for multipartite quantum correlations. This measure has been obtained by suitably recasting the standard quantum discord in terms of relative entropy and local von Neumann measurements [as given by Eq. (19)]. In particular, our measure is a systematic extension of the original approach for quantum discord as introduced in Ref. [3], reducing to it in the particular case of bipartite systems. Illustrations of its use have been provided for both the Werner-GHZ and the Ashkin-Teller spin chain. Further applications of GQD, such as the investigation of multipartite correlations in quantum computation and connections with entanglement (see, e.g., Ref. [29]), are left for future research.

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